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Summary Report of Consultants' Meeting

XML Schema for Atomic and Molecular Data

IAEA Headquarters, Vienna, Austria

26–27 August 2008

Prepared by

D. Humbert

International Atomic Energy Agency, Vienna, Austria

October 2008

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Abstract

Advanced developments in computer technologies offer exciting opportunities for new distribution tools and applications in various fields of physics. The convenient and reliable exchange of data is clearly an important component of such applications. Therefore, in 2003, the A+M Data Unit initiated within the collaborative efforts of the DCN (Data Centres Network) a new standard for atomic, molecular and particle surface interaction data exchange (AM/PSI) based on XML (eXtensible Markup Language). The schema is named XSAMS which stands for "XML Schema for Atoms Molecules and Solids". A working group composed of staff from the IAEA, NIST, ORNL and Observatoire Paris-Meudon meets biannually to discuss progress made on XSAMS, and to foresee new developments and actions to be taken to promote this standard for AM/PSI data exchange. Such a meeting was held on 26, 27 August 2008, and the discussions and progress made in the schema are considered within this report.

October 2008

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IAEA Consultants' Meeting: XML Schema for Atomic and Molecular Data

26–27 August 2008, IAEA Headquarters, Vienna, Austria

Present

Mr D. Humbert, IAEA (*Scientific Secretary*)

Mr R.E.H. Clark, IAEA (*Opening of the meeting*)

Attendees:

Ms M-L. Dubernet (France)

Mr N. Moreau (France)

Ms E. Roueff (France)

Mr Yu. Ralchenko (United States of America)

Mr D.R. Schultz (United States of America)

Welcome and Opening of the Meeting

Participants were welcomed to the IAEA by Mr. Clark on behalf of the IAEA and the Nuclear Data Section. Minutes from the previous meeting and the agenda were adopted with no further modifications.

1. Presentation of the Schema at Various Technical Meetings

During the previous IVOA INTEROP meeting at Trieste in May, M-L Dubernet presented a proposal for an I3-FP7 project in support of XSAMS development and applications. I3-FP7 is a European initiative to support multidisciplinary projects in I-science. A large number of data centres and institutes from inside and outside the EU wish to join the project. Among participants from the EU are CDMS (France), Astrogrid (UK), VALD (Austria) and Chianti. Partnership is possible from outside EU as long as the project leader is European. The All-Russian Institute (Russia), NIST (USA) and CRAAMD (China) can also join the project. However, as an international organisation, the IAEA may not participate. Deadline to submit a proposal is 11 September 2008. Next I3-FP7 call for applications is planned in Spring 2010.

2. Review of Status of XML Schema

Participants agreed to name the schema **XSAMS** which stands for **X**ML Schema for **A**toms, **M**olecules and **S**olids.

XSAMS is in the final phase for release of version 0.1. As developers encountered minor problems during the development of XSAMS applications, an informal meeting took place in Paris, 9-10 July 2008. The purpose was not to review the physics within the schema, but to structure the schema to facilitate the work of developers. Agreements included:

1. Keep only one space name: XSAMS.

2. Elements and types are in UpperCamelCase; attributes in lowerCamelCase.
3. Every element and attribute has a type. A primary type with 2 attributes “sourceRef” and “methodRef” and 1 element “Comment” was introduced.

The existing schema was quickly reviewed. The following corrections were agreed upon:

- The schema is divided into files, and each file is self-consistent and valid – this approach imposes some redundant declarations in each file, for example “include typesAttributes.xsd”. Unnecessary “include” declarations have been removed.
- typesAttributes.xsd contains common types and attributes used in different xsd files. Types and attributes specific to one xsd file will be removed from typesAttributes.xsd and placed in their specific xsd file.
- Files have been renamed: typesAttr to typesAttributes, bibliography to sources, amdml to xsams.
- Marie-Lise presented the final form of the “molecularState” element. Quantum numbers are represented for most cases. A general description is possible as a list for an unsupported description of quantum numbers.
- Energy was renamed TransitionEnergy in the radiative part. The schema will be reviewed to ensure that any reference to “Energy” is unambiguous.
- Units: UNITSML from NIST will be used when available. A short list of units was proposed – to be reviewed later by D. Humbert and Yu. Ralchenko (see Annex 1).
- Methods “derived” and “observed” were added to the list.
- The “processes” element has three sections:
 - transition probabilities for radiative processes (*Data type*)
 - transition probabilities for non-radiative processes (*Data type*)
 - collisions (*DataXY type*)

Radiative and non-radiative processes are separate to reflect their own specificity. An unresolved issue is the possibility of replacing the name “Autoionization” by “NonRadiative”.

Action: Denis and Yuri to make the necessary changes and to post the xsd files on Google.

N. Moreau created a site on Googlecode for XSAMS. He explained the advantage in using such a site to facilitate schema maintenance. A demonstration was only partially successful as the IAEA does not allow connection using the SVN protocol. Further versions of the schema will be posted on this site (<http://code.google.com/p/xsams/>).

Unresolved issues

Some data representations are not included in the schema. The documentation should clearly mention the scope of the schema and what will be included in future releases. This requirement concerns isoelectronic series, isonuclear sequences, clusters, branching ratio, air broadening and Stark broadening. Band properties and solid spectroscopy do not comply with the current schema. The relevance to include isonuclear sequences should be checked within the atomic physics community.

3. Processes

The element “process” is complex for the collision part, with two optional elements: a user-defined element and a list of codes. D. Schultz presented a document (see Annex 2), listing

fundamental types for reactants (or products) and a list of processes. These processes can be combined to describe more complex processes. For example, a dissociative ionization will combine the two processes dissociation and ionisation. After discussion, the following decisions were agreed:

1. not implement a fundamental type for the reactants (or products),
2. implement this new list of processes,
3. properties for single reactant processes (transition probabilities, wavelength, etc.) were removed; they are not collisional processes. No list is needed for the Radiative and NonRadiative transitions, with the photon emission and the autoionisation being the possible processes,
4. keep the 3-letter IAEA code inside the schema.

Action: D. Humbert and Yu. Ralchenko to update the schema.

4. Documentation

An appropriate document will be provided with the first release of the schema:

- overview document *Yuri Ralchenko*
- sources *Dave Schultz*
- functions *Denis Humbert*
- methods *Denis Humbert*
- types and attributes *Yuri Ralchenko*
- statesAtoms *Yuri Ralchenko*
- statesMolecules *M-L Dubernet*
- statesSolids *Dave Schultz*
- processes
 - radiative *Evelyne Roueff*
 - non-radiative *Evelyne Roueff*
 - collisions *Denis Humbert*
- rules and conventions
- list of attributes and types

This report will be based on Latex, and IOVA document style will be used (e.g. M-L. Dubernet document). Marie-Lise provided the necessary files and templates. UML and documentation can be generated using XMLSPY, and gives a good overall structure to the document. As listed above, each main element will be a chapter. A chapter for the rules, syntax, conventions and naming adopted for XSAMS will also be included. Types and Attributes will be listed at the end of the document.

The draft report will be ready for review by the end of September, and will be posted at NIST before the ICAMDATA.

A logo is still required for XSAMS

5. Web sites, IAEA and NIST

The IAEA website needs minor updates:

- today's meeting is missing,
- include the name XSAMS and a logo,
- include the Russian VNIITF institute as a collaborator,
- change surface to solid.

XSAMS namespace and files will be at NIST – Yu. Ralchenko will propose a home page.

6. Namespace, Registry, DAL

These topics are still pending. Namespace and files will be at NIST.

7. ICAMDATA, China, October 2008

XSAMS will be publicized at the ICAMDATA with one oral session (Yu. Ralchenko), one common poster and a database demonstration.

The poster will include a short introduction, and applications of four different databases:

- IAEA ALADDIN
- NIST ASD
- BASECOL
- SPECTR-W3

Each database will include: a title for the request, the html output and the output xml file. Owing to the elapse time required by the Agency to produce a poster, material should be given to D. Humbert by the end of September.

8. Working Method, Working Plan and Time Schedule

Two important milestones are the release of version 0.1, and an announcement at the ICAMDATA. The next meeting is scheduled in Beijing on 27 October 2008. XML documents and reports will be posted on XSAMS Google group at (<http://groups.google.com/group/xsams>):

- 11 Sep 2008 Deadline for I3-FP7 proposal
- 30 Sept 2008
 - Draft document posted on AMDML Google group (*everyone*)
 - Material for the poster (*everyone*)
 - **Version 1.0 of the XML schema**
 - NIST web site (*Yu. Ralchenko*)
- 27 Oct 2008 XML meeting in Beijing, China
- **28-31 Oct ICAMDATA, Beijing, China**

9. Future Meeting

- 27 October 2008, before ICAMDATA, China

List of Units Proposed for XSAMS

Syntax has to be defined for multiplication, division, power. Some convention should also be defined for special characters such as micron. We will probably adopt the choice of UNITSML, once this schema becomes available. Proposed syntax are:

- cm-1,
- 1/cm, C.m (conflict with a.u.)
- cm** -1
- cm⁻¹
- cm⁻¹, cm^{-1}

XSAMS:

- syntax using “.” For multiplication and / for division is temporarily adopted
- No units with special characters are proposed
- a.u → au

Units' list

Energy

eV, keV, meV, MeV
 eV/u, keV/u, meV/u, MeV/u
 a.u. cm-1
 J, Ry, Hartree
 kJ/mol, kcal/mol
 K

Frequency

Hz, kHz, MHz

Length

m, cm, a.u., Å, nm

Angle

deg, rad, sr

Time

s, a.u.

Temperature

K, deg, eV, keV

Rate coefficient

m³/s, cm³/s

Cross sections

m², cm², b (barn), Mb, a.u.

Rate

s⁻¹

Probability, yield

unitless

Electric dipole moment
C.m, Debye, a.u.

Magnetic dipole moment
J/T, a.u.

Electric quadrupole moment
C.m², a.u.

Velocity
m/s, cm/s

Charge
C, e, a.u.

Mass
G, kg, a.u., amu

Flux (particle, energy, power)
Particle m⁻²s⁻¹, cm⁻²s⁻¹
Energy Jm⁻²s⁻¹, Jcm⁻²s⁻¹
Power Wm⁻²s⁻¹, Wcm⁻²s⁻¹,

Fluence
Particle m⁻², cm⁻²
Energy Jm⁻², Jcm⁻²
Power Wm⁻², Wcm⁻²,

Arbitrary unit

XSAMS Reactant and Process Codes

Version 0.1

26 August 2008

Introduction

In order to facilitate searching and sorting of XSAMS files or blocks of data within a file, a classification scheme is defined to provide standard definitions for the atomic, molecular, and solid *fundamental reactants* (e.g., an atom or photon) for which data are given and for the *fundamental process* that is being described (e.g., reflection of a particle from a surface or the excitation of an atomic state).

The reactant and process codes are “fundamental” in that they do not define the particles and reactions to a great degree of detail – this is carried out by specific elements of the overall schema. Rather, they provide a high level identification that can be used to aggregate similar data or provide a simple search point.

Reactant Codes

The following table defines the fundamental reactant codes. As an example of the use of these codes, suppose that the author of an XSAMS file wishes to provide data for an electron-impact process. The reactant code provides a tag that can be searched in order to quickly identify any available files for electron-impact. Combining this code with other reactant codes allows a more complete definition of the entities involved in the same manner as does the addition of a process code, as defined below.

Reactant Code	Full Name	Description
phot	Photon	A particle of light of any wavelength, e.g., IR photon, x-ray, etc., or polarization
elec	Electron	An electron of any energy or spin
posi	Positron	A positron of any energy or spin
atom	Atom	Any atom of the periodic table
atoi	Atomic ion	An ion of any charge state of any atom of the periodic table, e.g., a proton, Ar ¹²⁺
mole	Molecule	Any molecule, e.g., CH ₄ , in any electronic, vibrational, or rotational state
moli	Molecular ion	An ion of any molecule, e.g., H ₂ ⁺ , in any electronic, vibrational, or rotational state
surf	Surface	A material surface of any composition and structure, e.g., a monolayer of oxygen on an aluminum surface, the surface of a dust grain, etc.
sol	Solid	A bulk solid of any composition and structure, e.g., a block of stainless steel

Process Codes

The following table defines the fundamental reactant codes. As for the reactant codes, the process codes embody a high level description and a much more complete definition of the process to which data pertain is contained in the elements of the full schema. The codes are intended for use with any reactant code as well. For example, a single process code can be used to describe elastic scattering involving electrons colliding with an atomic ion or a photon reflecting from a surface. These can be recognized (parsed) as different because of the reactant codes - the elastic scattering of an electron from an atomic ion involves reactant codes “elec” and “atoi” while as the elastic scattering of a photon from a surface involves “phot” and “surf.”

This approach has been adopted not only for economy, but because an exhaustive list of processes involving elementary particles, atoms, molecules, and solids is not judged to be possible. Even if possible, adoption would be cumbersome in that some non-intuitive coding would be necessary, for example, to encode inverse bremsstrahlung, sublimation of water from a dust grain, production of an atomic inner shell vacancy with a subsequent Coster-Kronig decay, etc.

Multiple process codes can be given in order to build more complex descriptions from the fundamental processes, e.g., charge transfer – ionization in ion-atom collisions could be described by the code for ionization (liberation of an electron from the target or projectile to the continuum) and the code for charge transfer (the transfer of an electron from one collision partner to another). This combining of individual codes avoids the need for a code for all possible combinations of processes that are at least relatively common, e.g., dissociative recombination simply has the codes for dissociation and for recombination. Other examples of combinations of codes are given in the final table.

Process Code	Process Name	Description
prop	Property	Properties of fundamental reactants, i.e., atoms, molecules, etc., e.g., wavelengths, transition probabilities, line widths, interatomic potentials, etc.
phem	Photon emission	Emission of a photon or photons from a reactant (e.g., atom, molecule, surface), fluorescence
phab	Photon absorption	Absorption of a photon or photons from a reactant (e.g., atom, molecule, surface)
phsc	Photon scattering	Scattering of a photon or photons by a reactant
elas	Elastic Scattering	Scattering of one reactant from another without change of state or energy, including related processes such as momentum transfer
inel	Inelastic Scattering	Scattering of one reactant from another with change of state or energy. This code is provided in case none of the other specific inelastic codes are applicable or appropriate (e.g., energy or spin transfer reactions, projectile energy loss)
exci	Excitation	Excitation from a lower to higher state of any fundamental reactant, e.g., electron-impact excitation of an atom, photoexcitation of a molecule to a higher ro-vibrational state
deex	De-excitation	Induced or spontaneous transition from a higher state to a lower state, e.g., vibrational de-excitation in atom-diatom scattering
ioni	Ionization	Removal of an electron from any reactant the ends up in the continuum
tran	Charge transfer	Transfer of an electron from one “centre” (atomic ion, atom, molecule, etc.) to another
exch	Electron exchange	Exchange of an electron (most commonly in electron-impact processes) with another electron
reco	Recombination	Capture of an electron by an atomic or molecular ion, e.g., in dissociative recombination, dielectronic recombination, or radiative recombination
elat	Electron attachment	Formation of a negative ion by electron attachment
eldt	Electron detachment	Removal of the weakly bound electron of a negative ion by photon impact or collision with another particle such as an electron or surface
asso	Association	Association of two (or more) reactants, typically neutrals, collisionally, or radiatively

diss	Dissociation	Splitting of two (or more) reactants e.g., via electron-impact of a molecule, photodissociation, molecular break-up on a surface
intr	Interchange	Exchange of a heavy particle (atom, ion) in a reaction, e.g., $D + H_2 \rightarrow DH + H$
chem	Chemical reaction	Exchange of atoms or groups of atoms in chemical reactions, e.g., $C + 2 O \rightarrow CO_2 + \text{heat}$
sure	Surface: reflection	The elastic or inelastic reflection of a reactant from a surface
suem	Surface: emission or erosion	Any form of erosion of a surface, e.g., physical or chemical sputtering, etching, sublimation, emission of particle or macroscopic pieces, desorption, secondary electron emission
sudp	Surface: deposition	Absorption of particles by a surface, sticking, surface implantation
such	Surface: change	Change of the composition or properties of a surface induced by any reactant
sope	Solid: penetration – energy change	Penetration of a reactant into a solid, characterized by the change of energy, e.g., stopping, straggling, energy loss, range, charge state equilibrium
sops	Solid: penetration - structure	Penetration of a reactant into a solid, characterized by the change of structure, e.g., trapping, diffusion, deep implantation

The following table gives examples of the use of the fundamental process codes to describe more complex but still common processes. Some simply fall within the broad scope of one of the fundamental codes, and others can be described by use of multiple codes.

Under Construction

Common Process Name	Process codes	Description
Penning ionization	asso + ioni	Association of atoms with ionization
Transfer ionization	tran + ioni	Charge transfer between and ion and an atom, for example, with ionization
Transfer excitation	tran + exec	Charge transfer with excitation
Stripping	ioni	Ionization of the projectile in a collision of an ion or atom with an atom, molecule, or solid
Dissociative recombination	diss + reco	
Dielectronic recombination	reco	
Auger ionization	exci + ioni	
Spin-flip	inel	
photoionization	oni	
Three-body recombination	reco	
Superelastic scattering	inel	
Surface catalysis	sure + chem	
Stark shift		
Line broadening		
Bremsstrahlung		
Compton scattering		
Atomic oscillator strengths	prop, phot + exci	

Notes: photo-assisted processes, or processing in electromagnetic fields?

IAEA Consultants' Meeting: XML Schema for Atomic and Molecular Data

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26–27 August 2008, building-A, floor-23, room-11 (A2311), IAEA Headquarters, Vienna, Austria

MEETING AGENDA

Tuesday, 26 August

09:00 Opening, Bob Clark

Morning

1. Last meeting minutes review and adoption of the agenda
2. Reports on presentation of the schema to various technical meetings if any
3. Paris Meeting 9-10 July
4. Schema name: XSAMS?
5. Review of present “XSAMS” status

- New structure, introduction of types *Nicolas*
- Overview *Yuri*
- Atomic data *Yuri*
- Solid *Dave*
- Molecular data *Marie-Lise*
- Processes
 1. Radiative processes *Evelyne*
 2. Autoionization *Denis, Bob*
 3. Collisions *Denis, Bob*
- Biblio *Dave*
- Functions, methods *Denis*
- Types and attributes *Yuri*

Afternoon

6. Classification of processes, *Dave*
 - a. Atomic and molecular collisions
 - b. Particle surface interactions
7. Comments, corrections, new developments and unresolved issues from last meeting:
 - structure consistency, rules: draft document (*Denis*)
 - units, link with UNITSML
 - isoelectronic series, isonuclear sequences, quantum defects, average atom
 - isotopes

Estimated end of first day 17h

Wednesday, 27 August

09:00 Meeting Continued

Morning

8. XSAMS applications
 - ASD, *Yuri*
 - ALADDIN, *Denis*
 - BASECOL, *Marie-Lise*
9. Web site: IAEA (*Denis*), NIST (*Yuri*)
10. Draft document, *All*
11. Space name
12. Data Access Layer (*pending item*)
13. XSAMS web registry (*pending item*)

Afternoon

14. Collaboration
15. Work plan and milestones
 - a. Version 1.0
 - b. ICAMDATA, posters and invited paper
 - c. Dates for next meetings

Estimated closing time 16h

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